Flux String in Quantum Billiards with Two Particles

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Abstract

We examine the quantum motion of two particles interacting through a contact force which are confined in a rectangular domain in two and three dimensions. When there is a difference in the mass scale of two particles, adiabatic separation of the fast and slow variables can be performed. Appearance of the Berry phase and magnetic flux is pointed out. The system is reduced to a one-particle Aharonov-Bohm billiard in two-dimensional case. In three dimension, the problem effectively becomes the motion of a particle in the presence of closed flux string in a box billiard.

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The quantum billiard problem has been instrumental in revealing non-trivial features of seemingly simple systems with minimal degrees of freedom. As a consequence, unlike real-world billiards, quantum physicists' version of the billiard problem has only one particle moving within a walled boundary. The dynamics is controlled by the shape of the boundary, and by optional obstacles placed inside the billiard [1–5]. The formulation of zero-size obstacle [6,7] offers a possibility to go beyond this limitation, since it can be thought of as the second particle with infinitely heavy mass.

In this Letter, we consider the quantum mechanics of two and three dimensional systems consisting of two particles, one heavier than the other, interacting through a contact force, and confined in a walled rectangular boundary. Adopting the adiabatic separation of fast motion of the light particle and slow motion of the heavy one, we can formulate the problem in two steps. Namely, we first solve the motion of the light particle with the location of the heavy particle fixed, then calculate the effective Hamiltonian for the heavy particle using the eigenstates of the light particle. The first step yields a one-particle billiard problem in the presence of a pointlike scatterer, which has been the focus of several recent studies [7–10]. The identification of the Berry phase [11] in this one-particle billiard [9] then has an interesting ramification in the second step: The effective Hamiltonian for the heavy particle acquires a non-trivial vector potential which results in a field formally identical to the magnetism. We show that, in two dimension, this "magnetic" field appears as infinitely thin flux lines penetrating the billiard. Through a numerical example, we demonstrate that the flux lines have discernible effects both on the spectra and wave functions of the system. We also show that, in three dimension, the flux lines form closed strings which reside inside the billiard. Several examples of the flux string are displayed for a box billiard.

Let us suppose that two particles m and M each located at $\vec{r}$ and $\vec{R}$ interacting through a delta force are confined in a d-dimensional rectangular domain by a hard wall V_{wall}. We assume that M is substantially larger than m so that the motion of M can be treated adiabatically. The Hamiltonian describing the system is given by

$$H = \frac{\vec{P}^2}{2M} + h(\vec{R}) + V_{wall}(\vec{R}) \tag{1}$$

where $h(\vec{R})$ is a sub-Hamiltonian for the light particle which is given by

$$h(\vec{R}) = \frac{\vec{p}^2}{2m} + v\delta^d(\vec{R} - \vec{r}) + V_{wall}(\vec{r}). \tag{2}$$

For a fixed value of $\vec{R}$, this sub-system is known as the billiard with a pointlike scatterer [6–8]. As it stands, the resolvent of this sub-Hamiltonian is not well-defined for spatial dimension $d \geq 2$. However, in case of $d \leq 3$, the system can be made meaningful by redefining a coupling constant v in terms of renormalized coupling constant $\bar{v}$. Assuming that the $h(\vec{R})$ is handled with such proper renormalization procedure [8], we write the eigenvalue equation of $h(\vec{R})$ as

$$h(\vec{R}) \left|\alpha(\vec{R})\right\rangle = \omega_\alpha(\vec{R}) \left|\alpha(\vec{R})\right\rangle . \tag{3}$$

There are two types of solutions to this equation [9]. Let us denote the eigenvalue and eigenstate with $\bar{v} = 0$ (empty billiard) as ε_n and $|n\rangle$. The first, trivial type of solution exists when the delta potential is located on the node-line of unperturbed state;

$$\omega_\alpha = \varepsilon_n \quad \text{ if } \quad f_n(\vec{R}) = 0. \tag{4}$$

where $f_n(\vec{r}) = 0$ represents the node-line of the wavefunction $\langle\vec{r}|\, n\rangle$. The second, more generic type of solution of eq. (3) is obtained from the equation

$$\overline{G}(\vec{R}; \omega) - \frac{1}{\bar{v}} = 0 \tag{5}$$

where

$$\overline{G}(\vec{r}; \omega) = \sum_n \langle\vec{r}|\, n\rangle\langle n|\, \vec{r}\rangle \left[\frac{1}{\omega - \varepsilon_n} + \frac{\varepsilon_n}{\varepsilon_n^2 + 1}\right]. \tag{6}$$

is the inverse of transition matrix of the light particle m. If we assume that m stays at the adiabatic state $\left|\alpha(\vec{R})\right\rangle$ during the motion of M, we obtain an effective Hamiltonian governing the dynamics of M as

$$
\begin{aligned}
H_\alpha^{eff} &\equiv \left\langle \alpha(\vec{R}) \right| H \left| \alpha(\vec{R}) \right\rangle \\
&= \frac{1}{2M} \left(\vec{P} - \vec{A}_\alpha(\vec{R}) \right)^2 + U_\alpha(\vec{R}) + V_{wall}(\vec{R})
\end{aligned}
\tag{7}
$$

where the scalar potential U_α is given by

$$
U_\alpha(\vec{R}) = \omega_\alpha(\vec{R}), \tag{8}
$$

and the gauge potential (Mead-Berry connection) $\vec{A}_\alpha$ is given by [11,12]

$$
\vec{A}_\alpha(\vec{R}) = i \left\langle \alpha(\vec{R}) \right| \vec{\nabla}_R \left| \alpha(\vec{R}) \right\rangle . \tag{9}
$$

It is important that we choose normalized eigenstate $\left| \alpha(\vec{R}) \right\rangle$ as a single-valued function in the parameter space of $\vec{R}$. In some cases, $\vec{A}_\alpha$ can be made to be zero everywhere by redefining the phase of the $\left| \alpha(\vec{R}) \right\rangle$, but in general, this is not possible. When $\vec{R}$ makes an adiabatic cyclic motion, it acquires a geometric phase given by the circular line integral of $\vec{A}_\alpha$. The appearance of the vector potential is a consequence of the fact that this phase is non-zero. It is worth stressing that in the system considered here, the parameter space of slow variable is nothing but the coordinate space of heavy particle $\vec{R}$. Thus the vector potential $\vec{A}_\alpha$ resides in the coordinate space $\vec{R}$. The eigenvalue equation

$$
H_\alpha^{eff} \left| \Phi_{\alpha p} \right\rangle = E_{\alpha p} \left| \Phi_{\alpha p} \right\rangle \tag{10}
$$

gives the energy states of the whole system $E_{\alpha p}$ along with the eigenstate of the heavy particle $\left| \Phi_{\alpha p} \right\rangle$. They are indexed by two integers α and p each specifying the state for light and heavy particles.

We first concentrate on the case of two dimension. Since the Hamiltonian is real symmetric, the geometric phase is π when the path of the cyclic motion of $\vec{R}$ surrounds the diabolical point $\vec{R}^*$ [11,13], which is the point of degeneracy of the sub-Hamiltonian $h(\vec{R})$; namely $\omega_\alpha(\vec{R}^*) = \omega_{\alpha\pm1}(\vec{R}^*)$. Otherwise, the phase is zero. Since the quantity $\overline{G}(\vec{r};\omega)$ is a monotonous function of ω except at it's poles [8], the degeneracy can occur only between the solutions of eqs. (4) and (5). Therefore, location of $\vec{R}^*$ is determined by

$$f_n(\vec{R}^*) = 0 \quad \text{and} \quad g_n(\vec{R}^*) = 0 \tag{11}$$

where $g_n(R)$ is defined by

$$g_n(\vec{R}) \equiv \overline{G}(\vec{R}; \varepsilon_n) - \frac{1}{\bar{v}}. \tag{12}$$

In general, this equation has more than one solution for each degeneracy $\varepsilon_n = \omega_\alpha$. We write them as $\vec{R}^*_{\alpha j}$ $(j = 1, 2, \cdots)$. Because of the sign reversions around $\vec{R}^*_{\alpha j}$, single-valued representation of the eigenfunction $\left|\alpha(\vec{R})\right\rangle$ necessarily becomes complex even for the real symmetric Hamiltonian. There is a freedom to choose the gauge. We take the "maximally symmetric" choice around each $\vec{R}^*_{\alpha j}$;

$$\left|\alpha(\vec{R})\right\rangle = \exp\left(\frac{i}{2}\sum_j \varphi_{\alpha j}\right) N_\alpha(\vec{R}) \sum_n |n\rangle \frac{\left\langle n|\vec{R}\right\rangle}{\omega_\alpha(\vec{R}) - \varepsilon_n} \tag{13}$$

where $\varphi_{\alpha j}$ is an angle variable of $\vec{R}$ in the polar coordinate with its origin at $\vec{R}^*_{\alpha j}$, and N_α is a real normalization factor. From eqs. (9) and (13), we obtain

$$\vec{A}_\alpha(\vec{R}) = \sum_j \frac{-\vec{e}_{\varphi_{\alpha j}}}{2\left|\vec{R} - \vec{R}^*_{\alpha j}\right|} \tag{14}$$

where $\vec{e}_{\varphi_{\alpha j}}$ is a unit vector of the direction $\varphi_{\alpha j}$. We choose its direction such that $(\vec{R} - \vec{R}^*_{\alpha j}) \times \vec{e}_{\varphi_{\alpha j}}$ points to the positive z-axis in usual right-hand convention. The gauge curvature (or the "magnetic" field) $\vec{B}_\alpha$ is given by

$$\vec{B}_\alpha(\vec{R}) = \vec{\nabla} \times \vec{A}_\alpha(\vec{R}) = \sum_j (-\vec{n}_z)\pi\delta^2(\vec{R} - \vec{R}^*_{\alpha j}) \tag{15}$$

where $\vec{n}_z$ is the unit vector of the direction of z-axis. The problem is now turned into the motion of a particle M in the presence of infinitely thin lines of magnetic flux piercing through the billiard. This type of system is known as Aharonov-Bohm billiard [14,15]. Each flux line has the strength π, or $1/2$ in the unit of 2π which is usually adopted in the literature. This is known to give the anti-unitary symmetry to the system guaranteeing the correct global quantum properties such as level statistics. It is easy to see that the eigenvalues of the effective Hamiltonian, eq. (7) are unchanged under $\vec{n}_z \to -\vec{n}_z$, while the

phase of eigenfunctions changes. This means that the physics of a particle M is invariant under the reversion of the vector potential. In fact, for infinitely thin flux, the direction of $\vec{B}$ can be changed arbitrarily as long as it is off the billiard plane. This corresponds to the gauge transformation of the vector potential. Explicit calculation of eq.(7) with eq.(14) shows that the vector potential acts as centrifugal barrier with square inverse radial dependence around each diabolical points. That will effectively cause the wavefunctions to avoid the flux lines.

To illustrate our arguments, we show a numerical example. The billiard boundary is chosen to be a rectangle of size $[L \times 1/L]$ where $L = 1.1557$. The mass of the light particle is set to $m = 2\pi$, and the heavy particle $M = 5m$. The strength of the coupling is chosen to be $\bar{v} = 10$. In Fig. 1, the energy eigenvalue of the system is shown. In each of the energy levels, left side is the full calculation, and the right side is the calculation neglecting the effects of flux lines. The density profile of the eigenstates of the heavy particle $\left|\left\langle \vec{R} \,|\Phi_{\alpha p}\right\rangle\right|^2$ for selective α and p are depicted in Fig. 2, along with the location of the magnetic flux which is shown as black squares. The repulsive effect of the magnetic flux line is clearly visible.

We now turn to the three dimensional case. We consider a generic case of three-dimensional box-shaped domain in which unperturbed single-particle spectra have no degeneracies. The diabolical locations are determined by the same eq. (11) as in two dimensional case, but with $\vec{R}^*$ now representing a three dimensional coordinate vector. The condition, eq. (11) specifies a one-dimensional line in the space of $\vec{R}$. This is to be expected also from another perspective. Since the degeneracy is co-dimension two for real symmetric Hamiltonian, $\vec{R}^*$ cannot be the isolated points in the three-dimensional space of $\vec{R}$. Rather, it becomes a line of degeneracies. Clearly, the line cannot have the edge inside the billiard domain. Also, the line does not go through the domain wall, since this would mean that the unperturbed system has a degeneracy, which we have excluded in our assumption. The only possible configuration for the line of degeneracy, therefore, is the *closed string*. When one makes adiabatic circular motion of $\vec{R}$, the state of the sub-system $\left|\alpha(\vec{R})\right\rangle$ obtains a phase π if the circle is such that degeneracy strings pierce through its area odd number of times.

Otherwise, the geometric phase is zero. With the Stokes theorem, it is easy to show that the gauge potential $\vec{A}_\alpha$ whose circular line integral has such properties gives the flux $\vec{B}_\alpha$ which is non-zero only along the degeneracy string. Thus the string of degeneracy might be called the *flux string*. The strength of the flux $\vec{B}_\alpha$ along the string is 1/2 in the unit of 2π. Formally, it is given by

$$\vec{B}_\alpha(\vec{R}) = \left(\frac{1}{2}\right) \int d\vec{R}^S \delta(f_n(\vec{R}^S))\delta(g_n(\vec{R}^S))\vec{n}(\vec{R}^S) 2\pi \delta^3(\vec{R} - \vec{R}^S) \tag{16}$$

where $\vec{n}(R)$ is the direction vector of the flux string. As in dimension two, one can reverse the direction of $\vec{n}$ without changing the physics.

As in two dimension, the flux string in three dimension will have observable effects on the motion of the slow particle, and thus on the energy spectra of the system. Such calculation tends to become tedious for three dimension. Instead, in Fig. 3, we simply display the flux string for the system of two particles in a box of size $[L_x, L_y, 1/(L_x L_y)]$ where $L_x = 1.1557$ and $L_y = 1.0310$. The mass and the coupling constant are chosen to be $m = 2\pi$ and $\bar{v} = 10$ as before. It is evident that the flux strings possess the pictorial nature which is quite striking. We think that the impact is enhanced by the fact that these objects emerge from nothing more than two interacting particles in a box. If the observation of wave functions in a box becomes possible, these flux strings will be visible as the empty void of the probability distribution.

The magnetic flux string similar to the one found here has been predicted and discussed in the context of field theories. In elementary particle physics, it is known as *U(1) vortex* [16], and in cosmology as *cosmic string* [17]. It is quite conceivable that the actual experimental observation of magnetic flux string may be first realized at mesoscopic scale in a system similar to the one considered here. Further, the present study with a very simple setting suggests that, despite its exotic appearance, the flux string is ubiquitous in many-body quantum systems. We conclude that the quantum billiards acquire considerable richness with the introduction of more than one moving particle.

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FIGURES

FIG. 1. Energy level scheme of the eigenvalue equation eq. (10) with the effective Hamiltonian, eq. (7). The size of the rectangular boundary is set to $[1.15572, 0.86526]$. Other parameters are $m = 2\pi$, $M = 10\pi$ and $\bar{v} = 10$.

FIG. 2. The density profiles of the probability distribution of the heavy particle of the several selective eigenstates of eq. (10) for the rectangular billiard of $L = 1.15572$. the numbers in the figure refers to the quantum numbers (α, p).

FIG. 3. Flux strings found in the two particle billiard problem in a three dimensional box of the size $[1.1557, 1.0310, 0.8392]$. (a) $n = 2$, (b) $n = 3$, (c) $n = 4$, (d) $n = 5$, (e) $n = 6$, (f) $n = 7$, in eq. (11), respectively.

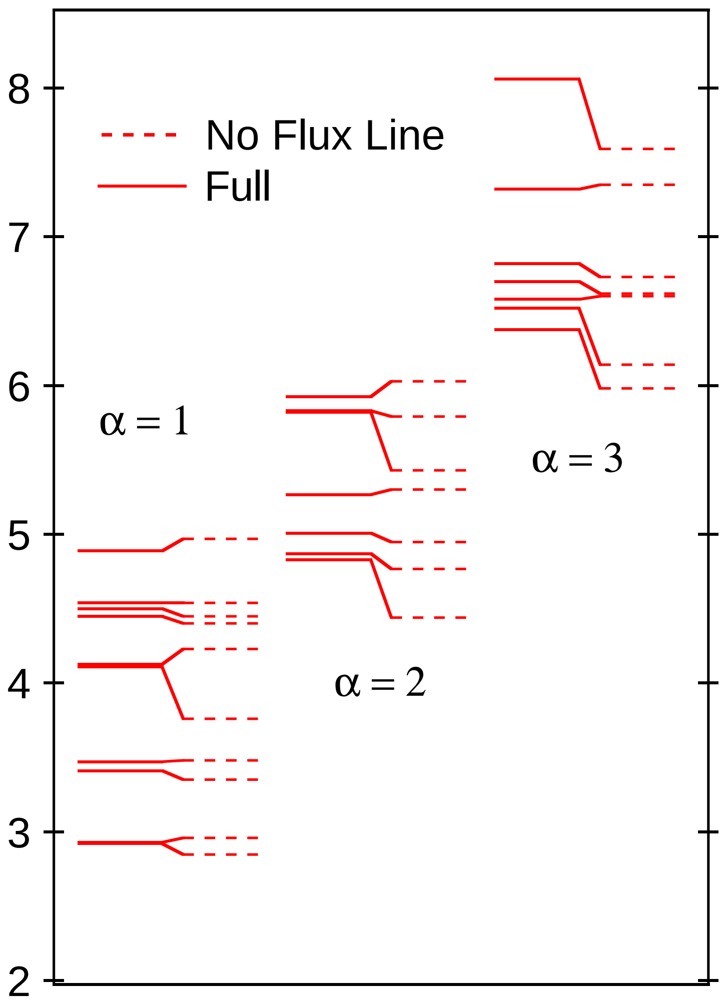

Fig. 1

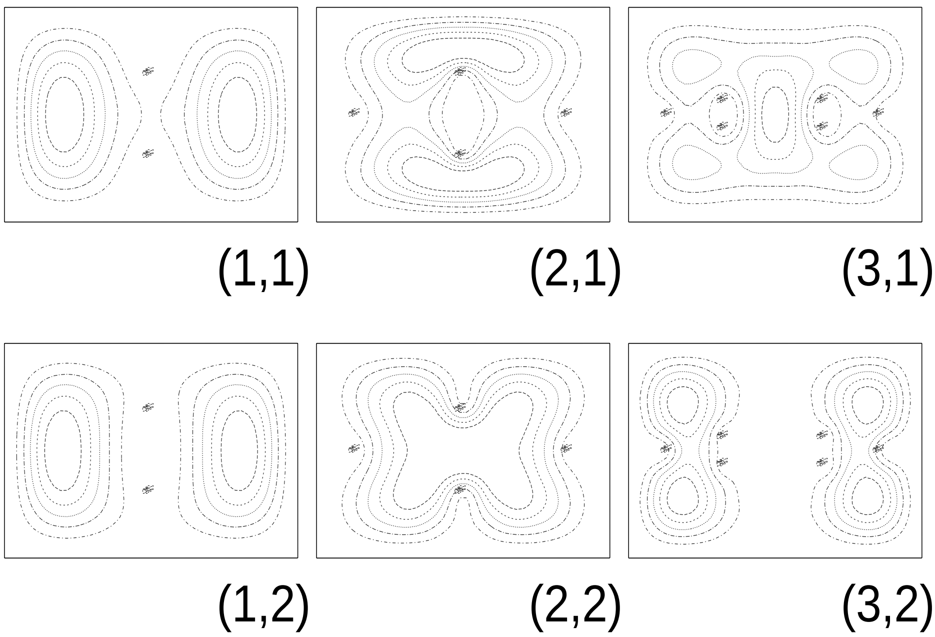

Fig. 2

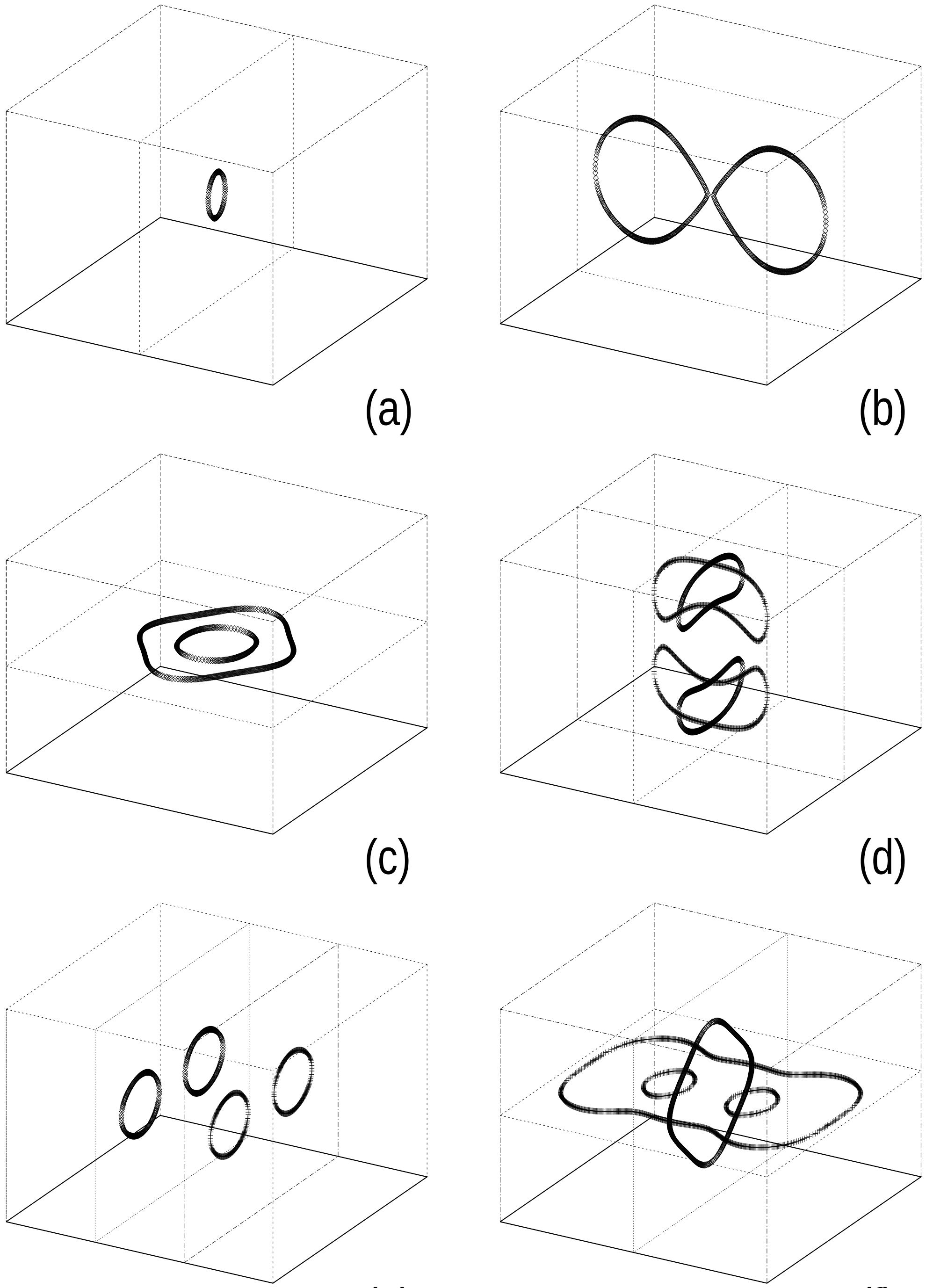

Fig. 3